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SURVEY OF APPROXIMATION PROCEDURES
FOR THE NUMERICAL SOLUTION OF
THE NEUTRON TRANSPORT EQUATION

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ABSTRACT

This report contains an evaluation of various methods
for the numerical solution of the stationary one-group
neutron transport equation. Emphasis is on those methods
which are applicable to transport calculations for multi-
dimensional heterogeneous reactor configurations under
realistic boundary conditions. In particular, attention
is focussed on the formulation aspects of these approxi-
mate procedures. The first part of the report deals with
synthesis techniques (spherical harmonics method, moment
methods), the second part with discrete ordinates techniques.

I. INTRODUCTION

In this report we present an evaluation of various methods for the
numerical solution of the stationary neutron transport equation, with
emphasis on those methods which are applicable in transport calculations
for multidimensional heterogeneous reactor configurations under realistic
boundary conditions. Extensive bibliographies on neutron transport have
been compiled and published by Rosescu[1*] in 1966 and by Hendry, et al.[2] in
1970. The present report covers a small area of the same field in greater
depth, with emphasis on the evaluation aspect, rather than the compilation
aspect. Specifically, we focus attention on the formulation aspects of
the various approximate procedures which have been proposed for the nu-
merical solution of the one-group transport equation. Procedures based
on the use of stochastic techniques (Monte Carlo methods) have been ex-
cluded, as they would easily justify a separate study.

In the multigroup formulation, the neutron transport equation is rep-
resented by a coupled system of linear integrodifferential equations for the
neutron flux, ψ,

$$\underset{\sim}{\Omega} \cdot \underset{\sim}{\nabla} \psi_g(\underset{\sim}{r},\underset{\sim}{\Omega}) + \Sigma_g^t(\underset{\sim}{r})\psi_g(\underset{\sim}{r},\underset{\sim}{\Omega})$$

$$= \sum_{g'=1}^{G} \int T_{g'g}(\underset{\sim}{r};\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}')\psi_{g'}(\underset{\sim}{r},\underset{\sim}{\Omega}')d^2\Omega' + S_g(\underset{\sim}{r},\underset{\sim}{\Omega}) \qquad g = 1\ldots G, \quad (1)$$

where G is the number of energy groups and g is the group index; $\psi_g(\underset{\sim}{r},\underset{\sim}{\Omega})d^3r\ d^2\Omega$ is the expected number of neutrons of energy group g in the volume element d^3r about $\underset{\sim}{r}$, whose velocities are directed in the element of solid angle $d^2\Omega$ about $\underset{\sim}{\Omega}$ ($|\underset{\sim}{\Omega}|=1$); Σ^t is the macroscopic total cross section, $T_{g'g}$ is the cross section for transfers from the energy group g' and direction $\underset{\sim}{\Omega}'$ to the energy group g and direction $\underset{\sim}{\Omega}$. In the g-th energy group, the source S_g is the sum of two contributions, one due to fission sources and another due to sources that are independent of the neutron flux in the reactor; so, instead of Eq. (1), we may write

$$\underset{\sim}{\Omega} \cdot \underset{\sim}{\nabla} \psi_g(\underset{\sim}{r},\underset{\sim}{\Omega}) + \Sigma_g^t(\underset{\sim}{r})\psi_g(\underset{\sim}{r},\underset{\sim}{\Omega})$$

$$= \sum_{g'=1}^{G} \int T_{g'g}(\underset{\sim}{r};\underset{\sim}{\Omega}\cdot\underset{\sim}{\Omega}')\psi_{g'}(\underset{\sim}{r},\underset{\sim}{\Omega}')d^2\Omega'$$

$$+ \frac{1}{4\pi}\sum_{g'=1}^{G} \chi_{g'g}(\underset{\sim}{r})(\nu\Sigma^f)_{g'}(\underset{\sim}{r})\phi_{g'}(\underset{\sim}{r}) + S_g^i(\underset{\sim}{r},\underset{\sim}{\Omega}) \qquad g = 1\ldots G. \quad (2)$$

In this equation, ϕ is the scalar flux, i.e., the integral of the neutron flux over all angles

$$\phi_g(\underset{\sim}{r}) = \int_{|\underset{\sim}{\Omega}|=1} \psi_g(\underset{\sim}{r},\underset{\sim}{\Omega})d^2\Omega. \qquad (3)$$

The fission process is assumed to be isotropic in the laboratory system of coordinates; Σ^f is the macroscopic fission cross section; $\nu_{g'}$ and $\chi_{g'g}$ are, respectively, the mean number of secondary neutrons and the fraction of secondary neutrons released in the group g due to a fission caused by a neutron of the energy group g'.

In the above equations, the coefficients Σ^t, $\nu\Sigma^f$ and χ, as well as the transfer kernels T are pointwise dependent upon the position $\underset{\sim}{r}$. To reduce the amount of data required for the numerical solution of the multigroup system of equations (2) it is commonly assumed that a reactor is

composed of a collection of homogeneous material regions. Thus, the coefficients Σ^t, $\nu\Sigma^f$, and χ and the transfer kernels T are no longer pointwise functions of position and we may consider them as region-wise constants.

The system of multigroup transport equations is coupled through the scattering and fission processes. Its solution must be obtained in an iterative manner. At each step, the equations are solved sequentially in the order of decreasing energy. That is, one writes Eq. (2) in the form

$$\underline{\Omega} \cdot \underline{\nabla} \psi_g(\underline{r},\underline{\Omega}) + \Sigma_g^t(\underline{r})\psi_g(\underline{r},\underline{\Omega})$$

$$= \int T_{gg}(\underline{r};\underline{\Omega}\cdot\underline{\Omega}')\psi_g(\underline{r},\underline{\Omega}')d^2\Omega' + S_g(\underline{r},\underline{\Omega}), \qquad g = 1\ldots G \qquad (4)$$

with

$$S_g(\underline{r},\underline{\Omega}) = \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \int T_{g'g}(\underline{r};\underline{\Omega}\cdot\underline{\Omega}')\psi_{g'}(\underline{r},\underline{\Omega}')d^2\Omega'$$

$$+ \frac{1}{4\pi} \sum_{g'=1}^{G} \chi_{g'g}(\underline{r})(\nu_{g'}\Sigma_{g'}^f)(\underline{r})\phi_{g'}(\underline{r}) + S_g^i(\underline{r},\underline{\Omega}).$$

One then considers Eq. (4) as an equation for ψ_g alone and solves assuming that S_g is a known function of the independent variables. This procedure is commonly known as the method of source iteration.

Thus, the solution of the multigroup system of transport equations (1) or (2) amounts to the solution of a sequence of equations of the type (4). Since the equations are all of the same form, it is sufficient to consider a single representative equation, which we write in the form

$$\underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r},\underline{\Omega}) + \Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega})$$

$$= \frac{\Sigma_s(\underline{r})}{4\pi} \int f(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}')d^2\Omega' + S(\underline{r},\underline{\Omega}). \qquad (5)$$

Observe that, if the one-group transport equation is written in the form (5), the source term S contains not only the independent sources, but

also the contributions due to in-scattering from other groups, as well as the contributions due to fission; it is assumed that S is a known function of its arguments. We will refer to the integral in the right member of Eq. (5) as the emission integral; f is called the phase function for single scattering, Σ_s the macroscopic scattering cross section.

The one-group transport equation is a first-order hyperbolic differential equation. Through every point $\underline{r}$ passes an infinite number of characteristics, each characteristic corresponding to a particular direction of the vector $\underline{\Omega}$. This is most easily seen if we write Eq. (5) in its characteristic or normal form,

$$-\left[\frac{\partial}{\partial s}\,\psi(\underline{r}-s\underline{\Omega},\underline{\Omega})\right]_{s=0} + \Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega})$$

$$= \frac{\Sigma_s(\underline{r})}{4\pi}\int f(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}')d^2\Omega' + S(\underline{r},\underline{\Omega}). \qquad (6)$$

We note that Eq. (6) may be integrated with respect to s to yield an integral equation for the neutron flux ψ,

$$\psi(\underline{r}-s\underline{\Omega},\underline{\Omega}) = \psi^o(\underline{r},\underline{\Omega})\,\exp\left(-\int_s^{s_o}\Sigma_t(\underline{r}-s'\underline{\Omega})ds'\right)$$

$$+ \int_s^{s_o} Q(\underline{r}-s'\underline{\Omega},\underline{\Omega})\,\exp\left(-\int_s^{s'}\Sigma_t(\underline{r}-s''\underline{\Omega})ds''\right)ds', \qquad (7)$$

where we have introduced the quantity $Q = Q(\psi,S)$,

$$Q(\underline{r},\underline{\Omega}) = \frac{\Sigma_s(\underline{r})}{4\pi}\int f(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}')d^2\Omega' + S(\underline{r},\underline{\Omega}),$$

which will be called the augmented emission integral.

Of course, Eqs. (5), (6), and (7) are equivalent and each of them may be used as the starting point for the formulation of approximation procedures for the numerical solution of transport problems. We will refer to Eq. (5) as the transport equation in *standard form*, to Eq. (6) as the transport equation in *normal form* and to Eq. (7) as the transport equation in *integral form*.

Before the advent of computers, the numerical investigations of problems of neutron transport (and of the related field of radiative transfer) were of a highly analytical nature. The symmetry of the problems was such that an appropriate description could be given in terms of an equation involving only one spatial and one angular variable (infinite slab, sphere with complete rotational symmetry). The numerical procedures were either synthesis techniques based on the use of Legendre polynomials or discrete ordinates techniques based on the use of Gauss-Legendre quadrature formulae. An account of these early approximation procedures may be found in the monographs of Chandrasekhar[3] and Davison.[4]

With the advent of computers, the emphasis in the numerical study of transport problems shifted to the use of low-order finite differencing techniques. Many computer programs for the solution of one-dimensional transport problems were developed; a survey as of 1958 has been given by Bareiss.[5] More recently, Greenspan, Kelber, and Okrent[6] have collected a number of survey articles on computational methods in reactor physics; two of these articles[7,8] deal with methods for solving the one-group transport equation. The present report supplements these sources of information.

Methods for solving the transport equation can be classified either as *synthesis techniques* or as *discrete ordinates techniques*. In a synthesis technique, the independent variables--$\underset{\sim}{r}$ = (x,y,z) and $\underset{\sim}{\Omega}$ = $(\Omega_x, \Omega_y, \Omega_z)$, with $|\underset{\sim}{\Omega}|$ = 1--are split into two disjoint sets and the dependent variable, ψ, is written as a linear combination of products of two functions defined over each of the disjoint sets of independent variables; one of these functions is assumed to be known (*trial function*), the other unknown (*coupling function*). The standard example of a synthesis technique is provided by the spherical harmonics method,[8] in which the trial functons are surface harmonics in $\underset{\sim}{\Omega}$ and the coupling functions depend on the spatial variables only. Other moment methods also fall in the category of synthesis techniques. In a discrete ordinates technique, a set of discrete directions $\{\underset{\sim}{\Omega}_k\}$ is chosen for the angular variable and the neutron flux $\psi(\underset{\sim}{r}, \underset{\sim}{\Omega})$ is replaced by a corresponding set of neutron

fluxes $\{\psi_k(\underline{r})\}$, with $\psi_k(\underline{r}) \equiv \psi(\underline{r}, \underline{\Omega}_k)$ for each k. The most common example of a discrete ordinates technique is provided by Carlson's discrete ordinates - S_N method,[7] in which the set of directions is chosen on the basis of considerations of invariance under certain rotation groups. Synthesis techniques are surveyed in Chapter II of this report, discrete ordinates techniques in Chapter III.

II. SYNTHESIS TECHNIQUES

A. Introductory Remarks

In this chapter we review those methods for obtaining numerical solutions of the transport equation which may be classified as synthesis techniques. The characteristic feature of a synthesis technique is that the independent variables $(\underline{r},\underline{\Omega})$ are split into two disjoint sets and that the dependent variable (the neutron flux, ψ) is written as a linear combination of products of two functions defined over each of the disjoint sets of independent variables; one of these functions is assumed to be known and is called a trial function, the other is assumed to be unknown and is called a coupling function.

Within the category of synthesis techniques one may further distinguish particular methods by means of various criteria; for example, (i) the form of the transport equation on which the approximation method is based--e.g., the standard form or the integral form of the transport equation; (ii) the method by which an approximate solution to the transport equation is determined--e.g., the collocation method, the least squares method, Galerkin's method or the method of weighted residuals; (iii) the particular splitting of the set of independent variables and the choice of the trial functions--e.g., as in the spherical harmonics method, the independent variables may be split in the spatial variables and the angular variables and the trial functions may be surface harmonics of the angular variables; (iv) the space in which the coupling functions are sought--e.g., a space of piecewise constant functions or a space of piecewise linear functions. Of course, the above scheme is by no means complete or unique, nor is it mathematically precise. Its purpose is to suggest various possible cataloguing schemes.

The next section (Section B) is a survey of recent advances in the spherical harmonics method. The spherical harmonics method is the most common synthesis technique for solving the transport equation. Some of the reasons for this are discussed in Section C. Also discussed in Section C are a generalized moment method for one-dimensional transport problems (slab, one-dimensional sphere and cylinder) due to Carlson, a moment method for two-dimensional transport problems in rectangular

(x,y)-geometry due to Lathrop and Demuth, and the relation between
moment methods and discrete ordinates methods for solving the trans-
port equation.

B. Spherical Harmonics Method

The spherical harmonics method is applicable in all geometries,
although the resulting equations become very unwieldy if the system
has few symmetry properties. A very detailed discussion of the spher-
ical harmonics method in slab geometry, spherical geometry, and
cylindrical geometry was given by Gelbard.[8] It is probably the best
reference available from the computational point of view. Also, it
contains an extensive bibliography, which covers most significant
articles through 1966.

1. Slab and spherical geometry

No new aspects of the spherical harmonics method in slab and
spherical geometry have appeared in the literature. DeBar[9] has sug-
gested recasting the system of differential equations for the Legendre
moments ψ_ℓ of the flux in "conservation form" (divergence form) and
then applying a spatial differencing technique in such a way as to pre-
serve the conservation properties. In the P_{2N-1} approximation there
are 2N conserved quantities of the form $E_n = \sum_{\ell=0}^{2N-1} \omega_\ell^{(n)} \psi_\ell$, n =
$-(N-1),\ldots,N$, where the weights $\omega_\ell^{(n)}$ obey certain recurrence relations.
One of the advantages of the conservation equation approach is, accord-
ing to DeBar, that it greatly limits the variety of spatial differencing
schemes one must consider. However, since DeBar does not support his
arguments with illustrative examples it is difficult to evaluate the
specific merits of this approach.

2. Cylindrical Geometry

The spherical harmonics method in cylindrical geometry is dis-
cusssed by Gelbard[8] for the case of an infinite cylinder. Recently,
Maeder[10] and Juillerat[11] formulated the spherical harmonics equations for
the case of a finite cylinder without and with axial variation of the
cross sections, respectively. The finite height is simply taken into
account by expanding the flux ψ in a Fourier series with respect to the
axial variable. The analytical methods for solving the spherical harmonic

equations (expansion in eigenfunctions and the method of Lie series, respectively) proposed by these two authors, are, however, less desirable from the numerical point of view--cf. the remarks by Gelbard [Ref. 8, Section 4.5].

3. Multidimensional geometries

As stated before, in multidimensional geometries the P_L equations become extremely complicated. A derivation of the P_L equations in general geometry will be found in Davison's monograph.[4] No numerical efforts have been reported beyond the P_3 approximation in two dimensions (TRIP programs). An attempt to generalize the double-P_L approximation to two dimensions was made by Gast,[12] who stipulated that a reduction to slab geometry by integration over lines parallel to one of the coordinate axes should produce the usual double-P equations with conical symmetry in the angular density. However, results obtained with the quadruple P_0 and P_1 equations for some transport problems in cylindrically symmetric systems showed a severe lack of cylindrical symmetry and, hence, suggest limitations in the applicability of this approach.

4. Truncation of the system of spherical harmonics equations

DeBar[13] has discussed the problem of truncating the spherical harmonic expansion. The common procedure consists of setting the expansion coefficient(s) of a given order equal to zero. The fact that this is not as accurate as possible was recognized by Davison.[14] For example, the fixed value of 1/3 for the diffusion coefficient which is obtained in the P_1 approximation, is not as accurate as the value obtained in asymptotic transport theory. Davison and later, independently, Pomraning[15] proposed a truncation procedure for the transport equation in slab geometry which, in the spherical harmonics approximation of order L, consists of making the Lth order Legendre polynomial expansion coefficient proportional to that of order (L-2). The constant of proportionality can then be chosen in such a way that the result becomes exact in the special limit desired. In a subsequent paper, Pomraning[16] gave an *ad hoc* generalization of this procedure for the transport equation in three-dimensional geometries. However, as was shown by DeBar,[13] this generalization fails because the particular truncation technique is valid only for the one-dimensional transport equation in slab geometry.

Taking an expansion of the angular flux in terms of the trace-less symmetric tensors $\underset{\approx}{p}^{i_1 \cdots i_\ell}(\underset{\sim}{\Omega})$ generated by $\underset{\sim}{\Omega}$, DeBar assumes that, in the spherical harmonics approximation of order L with L = 2N-1, the truncation expression shall be a linear combination of the first deriva-tives with respect to space (and time, in the case of the time-dependent transport equation) of all tensor coefficients of rank up to (2N-1). Linear combinations of the tensor coefficients themselves are excluded; one reason for this is that, otherwise, the truncation formula would be inconsistent in cases where the density is independent of space (and time). The coefficients in the linear combination of the first deriva-tives of the tensor coefficients--which, in general, are tensors too-- are taken to be scalar multiples of products of the metric tensor.

Thus it is shown that the most general linear truncation formula is in fact a *differential* formula, which is uniquely determined up to a scalar parameter. It is of the form

$$\underset{\sim}{\nabla} \cdot \underset{\approx}{\psi}^{(2)} = \alpha_o \underset{\sim}{\nabla} \psi^{(o)} \qquad \text{for N=1,}$$

$$\underset{\sim}{\nabla} \cdot \underset{\approx}{\psi}^{(2N)} = \alpha_{2N-2} \left[\underset{\sim}{\nabla} \underset{\approx}{\psi}^{(2N-2)} - \frac{2}{4N-3} \underset{\approx}{g}^{(2)} \underset{\sim}{\nabla} \cdot \underset{\approx}{\psi}^{(2N-2)} \right] \qquad \text{for N=2,3,...,}$$

where $\underset{\approx}{\psi}^{(i)}$ denotes an expansion tensor of rank i, $\underset{\approx}{g}^{(2)}$ is the metric tensor (Kronecker delta tensor in Cartesian coordinates), and α is the scalar parameter; each term on the right hand side has the indices of $\underset{\sim}{\nabla} \cdot \underset{\approx}{\psi}^{(2N)}$ and is symmetrized with respect to them. The parameter α may be so adjusted, for example, that the spherical harmonics equations yield the proper value of the diffusion length.

From DeBar's analysis it is evident that the difficulties en-countered by Pomraning in his attempt to generalize the original trunca-tion procedure to other than slab geometries were due to the neglect of the tensor nature of the quantities involved.

5. Application of variational principles

There exist several variational principles which characterize the transport equation together with its boundary conditions. With respect to the spherical harmonics method we note that Davis[17] has used variational

principles to show that, under appropriate interface and boundary conditions, the solution of the transport equation with non-zero absorption cross section is, in a very specific sense, approached monotonically from above by the solutions of the odd-P_L equations and from below by the solutions of the even-P_L equations. Davis has utilized this "bracketing property" of the spherical harmonics method to find bounds for an escape probability in one instance, and for a disadvantage factor in another. We refer to the original paper for further details.

The variational principles used by Davis were based on the concept of even- and odd-parity fluxes. They yield upper and lower bounds for integrals of the form $<S^-,\psi> = \iint S(\underline{r},-\underline{\Omega})\psi(\underline{r},\underline{\Omega})d^3r\ d^2\Omega$, where ψ is the solution of the transport equation. The ideas of Davis were later generalized by Buslik,[18] who used variational principles based on the concept of the adjoint flux. Thus, Buslik was able to produce upper and lower bounds for integrals of the form $<S^*,\psi> = \iint S^*(\underline{r},\underline{\Omega})\psi(\underline{r},\underline{\Omega})d^3r\ d^2\Omega$ with S^* arbitrary, rather than with $S^*(\underline{r},\underline{\Omega}) = S(\underline{r},-\underline{\Omega})$. When spherical harmonics trial functions are used, it turns out that the even-parity components of the approximate $\psi(\underline{r},\underline{\Omega})$ are obtained from the solution of an odd-order P_L calculation with a source distribution $S_1 = \frac{1}{2}[S(\underline{r},\underline{\Omega}) + S^*(\underline{r},-\underline{\Omega})]$. Similarly, the odd-parity components of the approximate $\psi(\underline{r},\underline{\Omega})$ are obtained from the solution of an even-order P_L calculation with a source distribution $S_2 = \frac{1}{2}[S(\underline{r},\underline{\Omega}) - S^*(\underline{r},-\underline{\Omega})]$. Hence, only conventional P_L-calculations are required, which is an attractive feature of this method. These ideas were used by Buslik to calculate upper and lower bounds for regionwise absorption rates in a rectangular configuration under reflecting boundary conditions.

6. Interface and boundary conditions

The following authors deal specifically with interface and boundary conditions to be used in conjunction with the spherical harmonics method: Rumyantsev,[19] Federighi,[20] Dede and Bödy,[21] Toivanen,[22] and Davis.[23,24] Most of these references are included in Gelbard's survey article.[8] Since no new aspects have been reported, we refrain from any further discussion of boundary conditions.

7. Spherical harmonics method applied to the integral transport equation

In previous paragraphs it has been tacitly assumed that the spherical harmonics method is applied to the standard integrodifferential form of the transport equation. This is the most common procedure, but by no means the only one possible. In fact, the spherical harmonics method has been applied to an integral form of the transport equation by Church,[25] Aswad & Dalton,[26] and Carlvik.[27]

Church and Aswad & Dalton use the "first-flight homogeneous Green's function" to transform the integro-differential equation into an integral equation. That is, they first rewrite Eq. (5) in the form

$$\underline{\Omega} \cdot \underline{\nabla} \, \psi(\underline{r},\underline{\Omega}) + \Sigma_t \psi(\underline{r},\underline{\Omega}) = [\Sigma_t - \Sigma_t(\underline{r})]\psi(\underline{r},\underline{\Omega}) + Q(\underline{r},\underline{\Omega}),$$

where Σ_t is some constant. Then they use the Green's function of the streaming operator of the above equation to rewrite the transport equation in integral form. Thus, ψ satisfies the following equation

$$\psi(\underline{r},\underline{\Omega}) = \int d^3r' \int d^2\Omega' \, g(\underline{r},\underline{\Omega};\underline{r}',\underline{\Omega}')$$

$$\times \{[\Sigma_t - \Sigma_t(\underline{r}')]\psi(\underline{r}',\underline{\Omega}') + Q(\underline{r}',\underline{\Omega}')\}, \qquad (8)$$

where g is the solution of the differential equation

$$(\underline{\Omega} \cdot \underline{\nabla} + \Sigma_t)g(\underline{r},\underline{\Omega};\underline{r}',\underline{\Omega}') = \delta(\underline{r}-\underline{r}')\delta(\underline{\Omega}-\underline{\Omega}'),$$

subject to the boundary conditions imposed on the solution of the transport equation, Eq. (5). To eliminate the angular dependence, all quantities having angular dependence are subsequently expanded in surfac harmonics. Thus one obtains the following infinite system of equations,

$$\psi_{k\ell}(\underline{r}) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \int d^3r' \, g_{k\ell}^{mn}(\underline{r};\underline{r}') \left\{ [\Sigma_t - \Sigma_t(\underline{r}')]\psi_{mn}(\underline{r}') \right.$$

$$\left. + Q_{mn}(r') \right\} \qquad \begin{array}{l} \ell = 0,1,\dots \\ \\ k = -\ell, = \ell+1, \dots, \ell \end{array} \qquad (9)$$

where, for any function $f(\underline{\Omega})$, the angular moments $f_{k\ell}$ are defined by

$$f_{k\ell} = \int_{|\underline{\Omega}|=1} f(\underline{\Omega}) Y_{k\ell}(\underline{\Omega}) d^2\Omega \qquad \ell = 0,1,\ldots; \; k = -\ell,\ldots,\ell,$$

and

$$g_{k\ell}^{mn}(\underline{r};\underline{r}') = \int d^2\Omega \int d^2\Omega' g(\underline{r},\underline{\Omega};\underline{r}',\underline{\Omega}') Y_{k\ell}^*(\underline{\Omega}) Y_{mn}(\underline{\Omega}') .$$

The system of equations (9) is equivalent to the transport equation (5) and valid for any geometry.

The real difficulty with this approach is in the construction of the Green's function $g(\underline{r},\underline{\Omega};\underline{r}',\underline{\Omega}')$ and its angular moments $g_{k\ell}^{mn}(\underline{r};\underline{r}')$. In some cases, the infinite-medium Green's function can be used to generate the solution to a finite-geometry problem. This approach was successfully used by Aswad & Dalton for the case of a unit slab cell (two-medium problem) with reflecting outer boundaries. In general such an approach is not possible and one may have to rely upon the generation of the Green's function via Monte Carlo techniques. The latter approach was used by Church, also for the case of a unit slab cell. Finally, we remark that both Church and Aswad & Dalton assume that the moments $\psi_{k\ell}(\underline{r})$ are piecewise constant functions of position. Since the cross sections and other material properties of the system are regionwise constant, the integral over $\underline{r}'$ in the right member of Eq. (9) can then be written as a finite sum of integrals and the expression in the braces can be brought outside the integral. Thus, Eq. (9) yields a linear system of algebraic equations, the coefficients of which involve integrals of the angular moments of the Green's functions.

Carlvik's analysis is based upon the integral form of the transport equation. For vacuum boundary conditions, Eq. (7) reduces to the following equation,

$$\psi(\underline{r},\underline{\Omega}) = \int_0^\infty ds \; e^{-\tau(s)} Q(\underline{r}-s\underline{\Omega},\underline{\Omega}) ds, \qquad (10)$$

where $\tau(s)$ is the optical distance corresponding to s. An expansion in terms of surface harmonics is subsequently applied to Eq. (10). The

configurations considered by Carlvik are multilayered systems of homogeneous slabs, homogeneous concentric annuli or homogeneous concentric spherical shells. Hence, there is only one spatial variable (r, say) involved. A characteristic feature of Carlvik's method is the discretization of this spatial variable in such a way that in each homogeneous region the mesh points coincide with the nodes of a Gaussian quadrature formula. The integral equation (10) thus involves point-to-point transfer kernels and in the spherical harmonics approach it reduces to a linear system of algebraic equations of the form

$$\psi_{k\ell}(r_i) = \sum_{j=1}^{J} \sum_{n=o}^{\infty} \sum_{m=-n}^{n} G_{k\ell}^{mn}(r_i;r_j) V_j Q_{mn}(r_j), \tag{11}$$

where V_j is a volume (weight factor) associated with the ordinate r_j.

Again, the major difficulty is in the calculation of the transfer matrices $G_{k\ell}^{mn}(r_i,r_j)$. Carlvik was able to express them in terms of relatively simple integrals for the three configurations mentioned earlier, but only after a considerable amount of algebraic manipulation. The application of this approach seems therefore hindered by limitations similar to those encountered in the approach discussed earlier in this subsection.

C. Other Synthesis Techniques

In the foregoing analysis we have always assumed that the phase function for single scattering depends on the cosine of the scattering angle $(\underline{\Omega}\cdot\underline{\Omega}')$, rather than on the directions $\underline{\Omega}$ and $\underline{\Omega}'$ separately. The assumption is justified if the scattering medium is isotropic, which is normally the case. The assumption renders the transport equation at each point $\underline{r}$ invariant under the three-dimensional rotation group (rotation with respect to $\underline{\Omega}$). It is well known[28] that the spherical harmonics $Y_{\ell m}(\underline{\Omega})$ are identical with the representation coefficients $\mathcal{D}^{(\ell)}(\{\phi,\theta,\gamma\})_{mo}$ of the three-dimensional rotation group, where ϕ and θ are the azimuthal and polar angles of $\underline{\Omega}$, respectively, and γ is arbitrary $(\mathcal{D}^{(\ell)}(\{\phi,\theta,\gamma\})_{mo}$ is independent of γ). Thus, it is natural to attempt solving the transport equation by means of a synthesis technique in which the trial functions are spherical harmonics in the angular variable. In those geometries

in which only the polar angle θ plays a role (i.e., in infinite slabs and in spheres with full rotational symmetry), the relevant representation coefficients are $D^{(\ell)}(\{\phi,\theta,\gamma\})_{oo}$, which are independent of both ϕ and γ. The $D^{(\ell)}(\{\phi,\theta,\gamma\})_{oo}$ are, in turn, identical with the Legendre polynomials $P_\ell(\cos\theta)$ and, hence, in those geometries the natural approach to the solution of the transport equation is via an expansion in Legendre polynomials. Instead of Legendre polynomials in $\mu = \cos\theta$ one could also use simple powers of μ as trial functions; however, in so doing one loses the convenience of orthogonality relations and addition theorems.

1. Carlson's moments method

Carlson[29] has attempted to formulate a general moment method for the transport equation, in which the form of the angular representation of the flux may be conveniently chosen and may be tailored to suit the requirements of the specific problem under consideration. The essential feature is that the form of the moment equations is not affected by the particular representation of the flux. For example, in slab and spherical geometries, if one applies the moment operators $\tilde{M}_m = \frac{1}{2}\int_{-1}^{1} d\mu\mu^m$ (m = $0,1,\ldots,2N-1$) to the transport equation one obtains a set of $2N$ equations which involve the angular moments of ψ up to order $2N$. Then, one chooses a suitable representation for the angular variation of ψ; the representation may be in the form of a single polynomial function of degree $2N-1$ for the entire interval $-1 \le \mu \le 1$, or in the form of a piecewise polynomial function with $2N$ degrees of freedom. If one applies the same moment operators $\tilde{M}_m$ for m = $0,1,\ldots,2N$ to this representation a system of expressions for the angular moments of ψ up to order $2N$ in terms of the coefficients of the representation is obtained. By inverting this system one can solve for the coefficients in terms of the moments and, thus, express the angular moment of order $2N$ in terms of the angular moments of order m = $0,1,\ldots,2N-1$. Substituting this expression into the system of moments equations one obtains a system of $2N$ equations involving the angular moments of ψ up to order $2N-1$, which can then be solved without further approximations. A similar method can be worked out for the transport equation in cylindrical geometry, in which case one uses the moment operators

$\tilde{M}_{\ell m} = \frac{1}{\pi} \int_0^1 d\xi \int_0^\pi d\omega \, \xi^\ell \mu^m.$ If $\ell + m < n$, the number M of moments involved for a given order, n, of approximation is then given by $M = 2^d n(n+2)/8$, where d is the dimensionality (here d=1). (Notation: $\underset{\sim}{\Omega} = (\mu, \xi)$, $-1 \le \mu \le 1$, $0 \le \xi \le 1$; $\mu^2 = (1-\xi^2)\cos^2\omega$, $\eta^2 = (1-\xi^2)\sin^2\omega$, $0 \le \omega \le \pi$.) The generalized moments method has not really led to any new approximation procedure for the numerical solution of the transport equation. Its main virtue is that it has led to some insight into the structure of the discrete ordinates equations which had been established earlier by Carlson and co-workers on the basis of heuristic arguments. We will elaborate upon this observation in the next subsection.

2. Discrete ordinates equations which are equivalent to moments representations

As was first shown by Richtmyer,[30] it is possible to define discrete ordinates equations in one-dimensional slab geometry that are equivalent to the P_L equations (if the complexity of the phase function for single scattering is suitably restricted). By "equivalent" is meant that, under appropriate boundary conditions, the P_L equations evaluated at the discrete directions give the same solution as the discrete ordinates equations. This result was rediscovered, independently, by Goertzel[31] and Gast.[32] A similar result holds in one-dimensional spherical and cylindrical geometries, see Gelbard.[8] In the case of Carlson's generalized moments method outlined above, analogous equivalences can be established. In fact, it was shown by Carlson and Lathrop[7,33] that, in both one-dimensional slab and spherical geometry it is possible to define discrete ordinates equations that are equivalent to the generalized moments equations.

These equivalence relations show two things, viz., that instead of the moments equations, one may solve an equivalent set of discrete ordinates equations and that it is possible to select the set of discrete directions in such a way that the invariance of the transport equation under the rotation group is preserved. The equivalence appears to be lost if one goes beyond the slab and one-dimensional spherical and cylindrical geometries. This fact has important consequences for the discrete ordinates techniques. Apparently in multidimensional geometries it is not possible to choose the

set of discrete directions in such a way that the invariance of the trans-
port equation under the rotation group is preserved. At best, one can
choose a set of discrete directions which is invariant under a particular
group of transformations on the unit sphere. In that case, the discrete
ordinates equations will enjoy the same invariance property. We will come
back to this point in the next subsection when we discuss the ray effect in
discrete ordinates techniques.

3. A synthesis technique in (x,y)-geometry

In an attempt to solve the transport equation in rectangular
(x,y)-geometry by synthesis techniques, Lathrop and Demuth[34,35] were led
to explore the utilization of a biorthogonal set of polynomials in two
variables first examined by Didon.[36] If the medium under consideration is
infinite in the z-direction and if sources and cross sections are inde-
pendent of z, then the neutron flux ψ is independent of z. Now, let the
vector $\underline{\Omega}$ be represented by its direction cosines $(\Omega_x, \Omega_y, \Omega_z)$; with
$\Omega_x^2 + \Omega_y^2 + \Omega_z^2 = 1$. If the source term and the boundary conditions are even
functions of the angle $\phi = \arctan(\Omega_z/\Omega_y)$, then the neutron flux ψ is an
even function of Ω_z and, therefore, a function of $\mu = \Omega_x$ and $\eta = \Omega_y$ alone.
Thus, the transport equation can be put in the form

$$\mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \Sigma_t \psi(x,y,\mu,\eta)$$

$$= \frac{\Sigma_s}{4\pi} \iint \frac{d\mu' d\eta'}{\sqrt{1-\mu'^2-\eta'^2}} [f(\mu_o^+) + f(\mu_o^-)]\psi(x,y,\mu',\eta')$$

$$+ S(x,y,\mu,\eta), \tag{12}$$

where $\mu_o^\pm = \mu\mu' + (1-\mu^2)^{1/2}(1-\mu'^2)^{1/2} \cos(\bar\phi + \phi')$. The emission integral ex-
tends over the unit disk $\{(\mu',\eta'): \mu'^2 + \eta'^2 \le 1\}$.

Lathrop and Demuth introduced the polynomials $U_{nm}(\mu,\eta)$ and
$V_{nm}(\mu,\eta)$, which are, respectively, the two-variable analogs of the
Tschebyscheff polynomials $T_n(\mu)$ and the Legendre polynomials $P_n(\mu)$. They
are defined by the generating functions

$$G_1(z_1,z_2,\mu,\eta) \equiv \frac{1 - \mu z_1 - \eta z_2}{(1-\mu z_1-\eta z_2)^2 + (1-\mu^2 - \eta)(z_1^2+z_2^2)} = \sum_{n,m=o}^{\infty} U_{nm}(\mu,\eta)z_1^n z_2^m \tag{13}$$

and

$$G_2(z_1,z_2,\mu,\eta) \equiv (1-2\mu z_1-2\eta z_2+z_1^2+z_2^2)^{-1/2} = \sum_{n,m=o}^{\infty} V_{nm}(\mu,\eta)z_1^n z_2^m, \tag{14}$$

and satisfy a biorthogonality relation of the form

$$\iint_{\mu^2+\eta^2\leq 1} \frac{d\mu\ d\eta}{\sqrt{1-\mu^2-\eta^2}} U_{nm}(\mu,\eta)V_{n'm'}(\mu,\eta) = \frac{2\pi}{2m+2n+1}\binom{m+n}{n}\delta_{nn'}\delta_{mm'}. \tag{15}$$

Furthermore, both polynomials U and V satisfy relatively simple recursion relations. By expanding the flux in terms of either the U or the V polynomials one obtains two infinite sets of partial differential equations for the moments ψ_{nm} of the flux ψ, which in this case are functions of the variables x and y. For the V-polynomial moments equations, Lathrop and Demuth were able to find an explicit connection with the usual spherical harmonics moments equations. They also showed that the V-polynomial moments equations in (x,y)-geometry reduce to the Legendre polynomial moments equations if either the x- or the y-dependence is eliminated.

In a subsequent paper, Lathrop[37] used the V-polynomial moments equations to investigate the existence of a set of discrete ordinates equations that are equivalent to the spherical harmonics equations (in the sense defined in the previous section). In one-dimensional geometries the equivalence is established by the truncation condition $P_n(\mu) = 0$ for n = 2N, so that the discrete ordinates are the zeros of $P_{2N}(\mu)$. The analogous situation in (x,y)-geometry is that $V_{nm}(\mu,\eta) = 0$ for n+m = 2N. Lathrop showed that the latter condition cannot be satisfied by any pair (μ,η) with $\mu^2+\eta^2 \leq 1$. Hence, it is not possible to define a set of discrete ordinates equations that are equivalent to the spherical harmonics equations and, thus, to preserve the invariance of the transport equation under the rotation group. As a consequence, any discrete ordinates technique applied to the transport equation in other than the one-dimensional

slab and spherical geometries, will lead to the so-called ray effect, i.e.,
irregularities in the flux pattern due to the preferential treatment of
certain directions. We will come back to this point in the next chapter
when the discrete ordinates techniques *per se* are discussed.

III. DISCRETE ORDINATES TECHNIQUES

A. Introductory Remarks

In this chapter we review those methods for obtaining numerical solutions of the transport equation which may be classified as discrete ordinate techniques. The characteristic features of a discrete ordinates technique are that a set of discrete ordinates $\{\Omega_k\}$ is chosen for the angular variable and that the neutron flux $\psi(\underline{r},\underline{\Omega})$ is replaced by a corresponding set of neutron fluxes $\{\psi_k(\underline{r})\}$, with $\psi_k(\underline{r}) \equiv \psi(\underline{r},\underline{\Omega}_k)$.

Within the category of discrete ordinates techniques one may further distinguish particular methods by means of various criteria, for example, (i) the form of the transport equation on which the approximation method is based--e.g., the standard form, the normal form, or the integral form of the transport equation; (ii) the nature of the spatial differencing technique--e.g., the diamond differencing technique of Carlson or a differencing technique based on the Euler-MacLaurin quadrature formula; (iii) the nature of the angular cubature formula for the evaluation of the emission integral--e.g., Carlson's S_N-formula or any cubature formula based on the use of Gauss's quadrature formula in one direction.

Again, this scheme is by no means unique or complete, nor is it mathematically rigorous. It serves only as a suggestion for various possible cataloging schemes.

In the present chapter we distinguish between discrete ordinates techniques based on the standard form of the transport equation, Eq. (5), and discrete ordinates techniques based on the normal form of the transport equation, Eq. (6). The former are surveyed and evaluated in Section B, the latter in Section C.

B. Discrete Ordinates Techniques Based on the Standard Form of the
Transport Equation

The use of discrete ordinates in transport theory was first sug-
gested by Wick in 1943, and extensively developed by Chandrasekhar.[3] The
technique was introduced not as a part of a numerical procedure for solv-
ing the transport equation, but rather as a step to facilitate the analyt-
ical work at some expense of accuracy. In other words, the discrete
ordinates method originated as a semi-analytical method. In the early
1950's it was realized that the method could also be used as a tool for
the numerical solution of the transport equation. Carlson and co-workers
at Los Alamos developed various versions of the discrete ordinates tech-
nique,[38,39,40] which were subsequently implemented in computer programs
for the numerical solution of the transport equation in one-dimensional
geometries (slab, sphere, infinite cylinder). Characteristically, they
were established on the basis of simple physical arguments and little
attention was paid to the mathematical aspects of the approximation pro-
cedure. We will return to this point in subsection 3 below.

1. Early results of Keller and Wendroff

The first authors who dealt with the question of convergence for
the discrete ordinates method were Keller[41,42,43] and Wendroff.[44] Their
investigations were limited to the transport equation for a homogeneous
slab ($-a \leq x \leq a$), in which the cross sections are constant: $\Sigma_t(x) \equiv \Sigma_t$
and $\Sigma_s(x) \equiv c\Sigma_t$. In the usual notation, the one-group transport equation
may then be written in the form

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \Sigma_t \psi(x,\mu) = \frac{c\Sigma_t}{2} \int_{-1}^{1} f(\mu,\mu')\psi(x,\mu')d\mu' + S(x,\mu). \qquad (16)$$

Keller and Wendroff proved the following theorem.

Let the errors in the approximate solution and in the quadrature
formula used for the evaluation of the emission integral be defined by

$$e_k(x) = \psi(x,\mu_k) - \psi_k(x)$$

and

$$\tau_k(x) = \int_{-1}^{1} f(\mu_k, \mu')\psi(x, \mu')d\mu' - \sum_{\ell=1}^{N} \omega_\ell f(\mu_k, \mu_\ell)\psi(x, \mu_\ell),$$

respectively. Then there exists a positive constant K such that

$$||e||_\infty \le K||\tau||_\infty \qquad \text{for} \qquad 0 \le c \le c_o \ (c_o > 1), \tag{17}$$

where

$$||e||_\infty = \max_k \ \max_x \ |e_k(x)|$$

and

$$||\tau||_\infty = \max_k \ \max_x \ |\tau_k(x)|.$$

Note that the theorem is a statement on error bounds for the discrete set of directions $\{\mu_k\}$; it does not state anything on error bounds for those values of μ which do not coincide with any of the μ_k. On the other hand, it is important to observe that no particular set of directions, nor a particular quadrature formula was adopted in the proof of the theorem.

The theorem of Keller and Wendroff is in accordance with intuition. It amounts to the fact that the discrete ordinates method converges pointwise and at least as fast as the quadrature formula (when the latter is applied to the exact solution). Apparently it passed almost unnoticed by those working on discrete ordinates methods and no further investigations of the mathematical aspects of the technique were reported in the literature.

2. Carlson's discrete ordinates-S_N method

Carlson and co-workers at Los Alamos continued a program to develop and extend various versions of the discrete ordinates technique, often with great ingenuity. However, their efforts were not adequately supported by firm mathematical arguments and, consequently, certain peculiar results of numerical calculations were encountered and could be explained

only on the basis of purely heuristic arguments. For an extensive survey of the state of the art as of 1967 we refer the reader to an article by Carlson and Lathrop.[7] There one finds a detailed discussion of various ways to derive the discrete ordinates equations, both in three-dimensional rectangular geometry and in curved geometries, as well as a discussion of the selection of discrete ordinates and angular quadrature schemes (S_N schemes). As a follow-up to this article we mention another article by the same authors, Lathrop and Carlson,[45] the first part of which deals with the discrete ordinates equation in one-dimensional spherical geometry and, in particular, with the spatial differencing aspect.

An article by Grant[46] contains the first more or less rigorous analysis of the relation between the discrete ordinates equations and the continuous transport equation. The analysis is performed for time-dependent problems in one-dimensional spherical geometry and in the terminology of radiative transfer, but is readily carried over to the case of neutron transport. We will now discuss the article in detail.

It is well known that the discrete ordinates technique by itself leads to systems of linear algebraic equations which contain more unknowns than there are equations. The additional equations necessary for the complete determination of all unknowns are called the auxiliary relations or difference relations. The standard difference relations are Carlson's step difference and diamond difference relations. The latter involve average function values along the edges of a mesh cell, as well as average function values over the interior of a cell. Grant viewed Carlson's difference relations as members of a class of difference relations which can be derived on the basis of (i) a principle of particle conservation for a finite cell in phase space, and (ii) an assumed flux shape within each cell in phase space. He analyzed the step and diamond difference relations as members of this class in terms of stability, positivity and truncation error. Specifically, he obtained the following results.

Let the one-group transport equation in spherical geometry be written in the form

$$L[\psi] = Q - \sum_t \psi, \tag{18}$$

where $\psi \equiv \psi(r,\mu)$ and the streaming operator L is defined by

$$L[\psi] = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \mu \psi) + \frac{1}{r} \frac{\partial}{\partial \mu} [(1-\mu^2)\psi];$$

let Ω represent a cell in phase space,

$$\Omega = \{(r,\mu): \quad r_i < r < r_{i+1}, \mu_{m-\frac{1}{2}} < \mu < \mu_{m+\frac{1}{2}}\};$$

and let Λ_Ω be the cell-averaged streaming operator,

$$\Lambda_\Omega[\psi] = \int_\Omega L[\psi]d\omega \Big/ \int_\Omega d\omega \qquad (d\omega = 4\pi r^2 dr\ d\mu).$$

Then the cell-averaged transport equation,

$$\Lambda_\Omega[\psi] = [Q - \Sigma_t \psi]_\Omega, \tag{19}$$

is identical with Carlson's discrete ordinates equation. The equation expresses the principle of particle conservation for the finite cell Ω in phase space. Let, furthermore, the flux shape in the cell Ω be such that

$$X_m \psi(r_{i+\frac{1}{2}}, \mu_{m+\frac{1}{2}}) + (1-X_m)\psi(r_{i+\frac{1}{2}}, \mu_{m-\frac{1}{2}}) = Y_m \psi(r_{i+\frac{1}{2}}, \mu_m) \tag{20a}$$

and

$$X_{i+\frac{1}{2}} \psi(r_{i+1}, \mu_m) + (1-X_{i+\frac{1}{2}})\psi(r_i, \mu_m) = Y_{i+\frac{1}{2}} \psi(r_{i+\frac{1}{2}}, \mu_m), \tag{20b}$$

where the constants X and Y are between 0 and 1. Then the system of linear algebraic equations (19) and (20) has a unique solution. Furthermore, Carlson's step difference scheme defined by choosing the auxiliary equations (20) with $X = Y = 1$ is unconditionally stable and its solution is positive whenever the sources and boundary fluxes are positive, and Carlson's diamond difference scheme defined by choosing the auxiliary

equations (20) with $X = \frac{1}{2}$, $Y = 1$ is unconditionally stable; in the latter case, nonnegativity of the solution cannot be guaranteed. Finally, there exists a value of $\theta_{i+\frac{1}{2}}$ $(0 < \theta_{i+\frac{1}{2}} < 1)$ such that, for a fixed angular mesh $(\mu_{m+\frac{1}{2}})$ and for $r_{i+\frac{1}{2}} = \theta_{i+\frac{1}{2}} r_{i+1} + (1-\theta_{i+\frac{1}{2}}) r_i$ if $\mu_{m+\frac{1}{2}} < 0$ and $r_{i+\frac{1}{2}} = (1-\theta_{i+\frac{1}{2}}) r_{i+1} + \theta_{i+\frac{1}{2}} r_i$ if $\mu_{m+\frac{1}{2}} > 0$, the truncation error of Eq. (19) is $O((\Delta r)^2)$. Similarly, there exists a value of θ_m $(0 < \theta_m < 1)$ such that, for a fixed spatial mesh (r_i) and for $\mu_m = \theta_m \mu_{m+\frac{1}{2}} + (1-\theta_m)\mu_{m-\frac{1}{2}}$, the truncation error of Eq. (19) is $O((\Delta\mu)^2)$. However, these choices of $\theta_{i+\frac{1}{2}}$ and θ_m do not lead to monotone operators and nonnegativity of the solution cannot be guaranteed.

There is one critical remark we wish to make with respect to Grant's analysis of the discrete ordinates equation. An assumption which is not clearly spelled out by Grant involves the evaluation of the cell-average of the first term of $L[\psi]$ - Eq. (2.9) of Ref. 46 - viz.,

$$\frac{\int_\Omega \frac{1}{r^2} \frac{\partial}{\partial r}(r^2\mu\psi)\,d\omega}{\int_\Omega d\omega} \equiv \frac{\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m-\frac{1}{2}}} [\mu A_{i+1}\psi(r_{i+1},\mu) - \mu A_i\psi(r_i,\mu)]\,d\mu}{V_{i+\frac{1}{2}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} d\mu}$$

$$= \mu_m \frac{A_{i+1}\psi(r_{i+1},\mu_m) - A_i\psi(r_i,\mu_m)}{V_{i+\frac{1}{2}}}. \tag{21}$$

There are two ways to evaluate this average.

(a) One applies the mean-value theorem twice to both terms in the numerator and obtains

$$\frac{\int_\Omega \frac{1}{r^2} \frac{\partial}{\partial r}(r^2\mu\psi)\,d\omega}{\int_\Omega d\omega} = \frac{\bar{\bar\mu}(r_{i+1})A_{i+1}\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \psi(r_{i+1},\mu)\,d\mu - \bar{\bar\mu}(r_i)A_i\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \psi(r_i,\mu)\,d\mu}{V_{i+\frac{1}{2}}\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} d\mu}$$

$$= \frac{1}{V_{i+\frac{1}{2}}} [\bar{\bar\mu}(r_{i+1})A_{i+1}\psi(r_{i+1},\bar\mu(r_{i+1})) - \bar{\bar\mu}(r_i)A_i\psi(r_i,\bar\mu(r_i))].$$

Here, we have explicitly indicated that the ordinates $\bar{\mu}$ and $\bar{\bar{\mu}}$ depend on the integrands involved and, therefore, on the particular values of r. To obtain the result of Eq. (21) one must require that (i) $\bar{\bar{\mu}}$ is independent of r, (ii) $\bar{\mu}$ is independent of r, (iii) $\bar{\mu}$ coincides with $\bar{\bar{\mu}}$. These requirements can only be met if one assumes that ψ does not vary across the cell (at least to the relevant order of approximation).

 (b) One rewrites the second expression in Eq. (21) as

$$\frac{\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \mu[A_{i+1}\psi(r_{i+1},\mu) - A_i\psi(r_i,\mu)]d\mu}{V_{i+\frac{1}{2}}\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \mu d\mu} \times \frac{\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \mu d\mu}{\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} d\mu} ,$$

which is equal to

$$\frac{1}{2}(\mu_{m-\frac{1}{2}} + \mu_{m+\frac{1}{2}}) \frac{A_{i+1}\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \psi(r_{i+1},\mu)d\frac{\mu^2}{2} - A_i\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \psi(r_i,\mu)d\frac{\mu^2}{2}}{V_{i+\frac{1}{2}}\displaystyle\int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} d\frac{\mu^2}{2}} .$$

One then applies the mean value theorem once to both integrals in the numerator and obtains the result

$$\frac{\displaystyle\int_\Omega \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\mu\psi)d\omega}{\displaystyle\int_\Omega d\omega} = \frac{\mu_{m-\frac{1}{2}} + \mu_{m+\frac{1}{2}}}{2} \frac{A_{i+1}\psi(r_{i+1},\tilde{\mu}(r_{i+1})) - A_i\psi(r_i,\tilde{\mu}(r_i))}{V_{i+\frac{1}{2}}}$$

This, in turn, reduces to the result in Eq. (21) if one requires that (i) $\tilde{\mu}$ is independent of r, (ii) $\tilde{\mu}$ coincides with the midpoint of the interval $[\mu_{m-\frac{1}{2}},\mu_{m+\frac{1}{2}}]$. In that case, one has automatically $\mu_m = \frac{1}{2}(\mu_{m-\frac{1}{2}} + \mu_{m+\frac{1}{2}})$ in Eq. (21). Again, these requirements are met only if one assumes that ψ does not vary across the cell (at least to the relevant order of approximation).

From Grant's analysis it is not clear whether the averaging procedure (a) or the averaging procedure (b) is used to derive Eq. (21). Yet, the distinction is important for the correct interpretation of the results: in procedure (a), $\psi(r_{i+1},\mu_m)$ and $\psi(r_i,\mu_m)$ stand for averaged fluxes *per se*, in procedure (b) they stand for weighted averaged fluxes, viz. weighted with respect to the direction cosine, μ; the latter (i.e., the weighted averages) are intimately related to the neutron current densities.

It is relatively straight-forward to verify that in the evaluation of the cell-average of the second term of $L[\psi]$ a procedure analogous to the procedure (a) above would lead to volume-averaged fluxes, whereas a procedure analogous to the procedure (b) above would lead to surface-averaged fluxes. In this case, the latter interpretation seems to be appropriate and has been adopted by Grant. For consistency one would, therefore, expect that the fluxes arising from the first term are weighted averages in the sense defined earlier.

From what has been said above with respect to the averaging procedures (a) and (b) it is obvious that the statement by Lathrop and Carlson (which is repeated by Grant) that the discrete ordinates equation is an exact conservation equation for a finite cell is not true unless one assumes a very specific behavior of the flux throughout the cell.

The analysis by Grant is a first attempt to put some rigor in the discrete ordinates technique for non-trivial (i.e., other than infinite slab) geometries. The complexity of the problem and the multitude of approximations one has to cope with left Grant with a feeling of dissatisfaction. He felt that the adopted equations were not based on a coherent underlying theory. In fact, from a later article by Grant and Hunt[47] we conclude that Grant has abandoned the discrete ordinates method entirely in favor of a method based on principles of invariance. It should be borne in mind, however, that Grant is interested primarily in radiative transfer problems of astrophysics. These problems are often adequately described in plane-parallel geometry, for which the principles of invariance are most easily formulated. In reactor physics, on the other hand, the transport problems are essentially three-dimensional and the application of the principles of invariance is practically impossible.

3. Two results for the discrete ordinates equations in (x,y)-geometry

The article by Grant discussed in the previous subsection dealt with the transport equation for spherically symmetric systems. We now discuss two results obtained by Davis, Hageman, and Kellogg,[48] which are relevant for the solution of the transport equation in two-dimensional systems with rectangular (x,y)-geometry. The equation reads, in discrete-ordinates form,

$$\mu_k \frac{\partial \psi_k}{\partial x} + \eta_k \frac{\partial \psi_k}{\partial y} + \Sigma_t \psi_k(x,y) = \Sigma_s \sum_{\ell=1}^{\tau} w_\ell f_{k\ell} \psi_\ell(x,y) + S_k(x,y) \qquad k=1 \ldots \tau, \qquad (22)$$

where ψ_k is the flux in the direction $\underset{\sim}{\Omega}_k$; μ_k and η_k are the x- and y-components, respectively, of $\underset{\sim}{\Omega}_k$; the w_ℓ are the cubature weights for the evaluation of the emission integral, $f_{k\ell}$ is the (nonnegative) phase function for single scattering from the direction $\underset{\sim}{\Omega}_\ell$ into the direction $\underset{\sim}{\Omega}_k$, and τ is the number of discrete directions in the upper hemisphere ($\Omega_z \geq 0$). Equation (22) is analyzed on a rectangular domain $R = \{(x,y): 0 \leq x \leq L_x, 0 \leq y \leq L_y\}$ under reflecting boundary conditions. It is assumed that the choice of the discrete directions $\underset{\sim}{\Omega}_k$ and the weights w_ℓ is compatible with this configuration. Equation (22) is discretized with respect to the spatial variables x and y by integrating over a mesh cell $(x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1})$. The result is a system of equations of the following form:

$$\mu_k \Delta y_j (V_{i+1,j}^k - V_{i,j}^k) + \eta_k \Delta x_i (H_{i,j+1}^k - H_{i,j}^k)$$

$$+ \Delta x_i \Delta y_j (\Sigma_{i,j}^t N_{i,j}^k - \Sigma_{i,j}^s \sum_{\ell=1}^{\tau} w_\ell f_{k\ell} N_{i,j}^\ell) = S_{i,j}^k$$

$$i = 1 \ldots I; \quad j = 1 \ldots J; \quad k = 1 \ldots \tau, \qquad (23)$$

where N is the average flux over a mesh cell and V and H are the average fluxes along the vertical (x constant) and horizontal (y constant) sides, respectively. The system of equations (23) must still be supplemented by the difference relations.

Davis et al. investigated the system of equations obtained by supplementing Eq. (23) by the diamond difference relations,

$$N_{i,j}^k = \frac{1}{2} (V_{i+1,j}^k + V_{i,j}^k),$$

$$N_{i,j}^k = \frac{1}{2} (H_{i,j+1}^k + H_{i,j}^k). \tag{24}$$

They proved the following theorem.

Under reflecting boundary conditions on the external boundary of R, the system of Eqs. (23) and (24) is singular. If the macroscopic absorption cross section $\sum_{i,j}^a = \sum_{i,j}^t - \sum_{i,j}^s \sum_{\ell=1}^{\tau} w_\ell f_{k\ell}$ is strictly positive for all i,j, then the system always has a solution. Moreover, the set of cell-averaged fluxes N is uniquely determined, although the fluxes averaged over the side of a mesh cell are not.

The same authors also investigated the central difference scheme which is obtained from Eq. (22) upon substitution of the bi-linear form

$$\psi_k(x,y) = a_k + b_k x + c_k y + d_k xy,$$

where the coefficients are determined by the values of the flux at the four corners of a mesh cell - $\psi_{i,j}^k$, $\psi_{i+1,j}^k$, $\psi_{i,j+1}^k$ and $\psi_{i+1,j+1}^k$. They proved that under reflective boundary conditions, the system of equations for the fluxes at the mesh points is singular and does not, in general, have a solution.

4. Truncation error analysis

The investigation of the truncation error in discrete ordinates methods, initiated by Grant, was continued and improved in a recent article by Reed and Lathrop.[49] These authors observe that the usual diamond difference scheme does not have a uniformly second order truncation error in curvilinear geometries. In fact, for one-dimensional spherical geometries the truncation error contains a term proportional to $(\Delta r)^2/r^2$, whereas $\Delta r \sim r$ near the origin of the coordinate system. The authors derive weighted diamond difference schemes for one-dimensional spherical and three-dimensional spherical and cylindrical geometries,

which have truncation errors that are uniformly of second order. The essence of the method is as follows.

In contrast to the standard diamond difference scheme, the phase space points $(r_{i+\frac{1}{2}}, \mu_m)$ where the dependent variable is considered to be evaluated, are not chosen at the centers of the phase space cells. Instead, it is assumed that

$$r_{i+\frac{1}{2}} = a_{i+\frac{1}{2}} \, r_{i+1} + (1 - a_{i+\frac{1}{2}}) r_i,$$

$$\mu_m = \tau_m \mu_{m+\frac{1}{2}} + (1 - \tau_m) \mu_{m-\frac{1}{2}},$$

and the parameters a and τ $(0 < a < 1, \ 0 < \tau < 1)$ are chosen so that the following three criteria are satisfied:

(i)   the truncation error is of second order in both variables simultaneously;

(ii)   the diffusion condition is satisfied, i.e., $\sum_m w_m \mu_m^2 = \frac{1}{3} \sum_m w_m$; in the case of a one-dimensional spherical geometry, the condition is automatically satisfied once the condition (i) above is satisfied;

(iii)   for a mesh symmetric about $\mu = 0$, the points μ_m are also symmetric.

Note that the angular intervals and the associated weights are given *a priori*; it is the angular direction μ_m within each cell which is to be chosen. Also note that the flux is still assumed to vary linearly across the cell (auxiliary equations).

The effectiveness of the weighted diamond difference scheme was illustrated on a k_{eff} calculation for a spherical critical assembly. When only spatial weighting was used ($\tau = \frac{1}{2}$) there was little effect on the accuracy of k_{eff}, but a spurious flux dip at the center was removed. When the angular weighting was used, the accuracy improved appreciably.

In heterogeneous systems there was no significant improvement over a standard S_8 calculation. Thus, as the authors point out, the

benefit of this approach is expected in two- and three-dimensional geometries, for which the cost of S_N calculations for $N \sim 8$ is large. It is hoped that the method of weighted diamond differencing with small N will give good accuracy.

5. The ray effect

The discrete ordinates approximation involves the evaluation of the transport equation at a discrete set of directions. Thus, the number of characteristic directions allowed for particle streaming is restricted and, consequently, the streaming contributions to the flux at a given position in the medium are limited to contributions from those characteristic directions in which sources are visible. This is the so-called *ray effect*, which was mentioned earlier in this report (see Chapter II, Section C, Subsections 2 and 3). The effect is in-herent to any discrete ordinates technique in multidimensional trans-port problems and gives rise to unrealistic flux depressions. An analysis of the ray effect was first given by Lathrop.[37]

In one-dimensional geometries (slab, sphere, infinite cylinder), it is possible to define discrete ordinates equations that are equivalent to moments equations. Here, "equivalence" must be understood in the fol-lowing sense: there exists a set of discrete directions such that the solution to the moments equations, when evaluated at these directions, is identical with the solution to the discrete ordinates equations based on this particular set of directions. The equivalence relation holds for the monomial moments equations[33] as well as for the Legendre polynomial moments equations.[30,31,32] With this observation in mind, Lathrop used the two-variables analogues of the Legendre polynomials (the V-polynomials introduced by Didon[36]) in an attempt to establish a set of discrete ordinates equations for the two-dimensional transport equation in (x,y)-geometry, which is equivalent to the set of moments equations based on these polynomials. As we already pointed out in Chapter II, Section C, Subsection 3, this attempt failed. However, Lathrop showed that the angu-lar moments obtained in the discrete ordinates - S_N approximation differ from the spherical harmonics moments (P_{N-1} approximation) through the presence of $\frac{1}{2}$ N cross moments which are not present in the spherical

harmonics approximation. Since the spherical harmonics method does
not exhibit the ray effect, the magnitude of the cross moments may be
considered as a measure of the ray effect in the discrete ordinates –
S_N equations.

Lathrop also showed that a set of discrete ordinates equa-
tions can be constructed from the discrete ordinates – S_2 equations
which is equivalent to the system of P_1-spherical harmonics equations
if the source term is modified to include derivatives of the first-
order cross moment Q – i.e., $Q(x,y) = 3 \sum_k w_k \mu_k \eta_k \psi_k (x,y)$. A general-
ization to higher order approximation schemes is possible provided
the angular quadrature sets will integrate polynomials of sufficiently
high degree correctly. For general N (N > 2) such sets have not been
found yet. Lathrop has pointed to some experimental evidence that
converting the discrete ordinates – S_N equations to the spherical
harmonics equations may destroy a favorable convergence property of
the former. That is to say, the discretization error for a discrete
ordinates – S_N approximation is not only of second order in the mesh
size; but, generally, the error bound constant is small as well. Thus,
the error is usually small, even for a relatively coarse mesh. This
favorable property may be lost in an approximation procedure based on
the spherical harmonics method, as the latter, like finite-difference
approximations to the diffusion equation, are generally rather sensi-
tive to the size of the mesh.

The ray effect is certainly a defect of the discrete ordinates
technique and, perhaps, a new approach is needed. Kaplan[50] has attempted
such an approach on the basis of variational principles.

6. Positivity vs. accuracy

The investigations discussed in the previous subsections dealt
primarily with the interplay of the spatial and angular approximations.
We now discuss another article by Lathrop[51] in which attention is
focussed upon the spatial approximation only. The author is concerned
with the problem of positivity vs. accuracy of various finite difference
schemes which have been suggested in the literature for the transport
equation in two-dimensional (x,y)-geometry.

The common factor of most finite difference schemes in dis-
crete ordinates methods is a postulated behavior of the neutron flux ψ
in each spatial mesh cell. For example, in some schemes it is postu-
lated that ψ is constant throughout a mesh cell, in other schemes that
ψ varies linearly across a mesh cell, etc. Then, at the next step of
the formulation of an approximation procedure, two broad classes of
procedures evolve depending on whether the standard form of the trans-
port equation or the normal form of the transport equation is used.
Both classes are discussed by Lathrop; however, we postpone a discus-
sion of the approximation procedures based on the normal form of the
transport equation until the next section (Section C). In the approxi-
mation procedures based on the standard form of the transport equation
one replaces the (integro-)differential equation by a system of balance
relations which are obtained by integrating the differential equation
over each spatial mesh cell. This system is subsequently supplemented
by a set of difference relations, as discussed earlier in the present
section (Subsection 2). One derives these difference relations by insist-
ing that fluxes with the postulated behavior in the mesh cell also satisfy
the balance relation for the cell. Thus, one obtains the step difference
relations by assuming ψ to be constant throughout the cell and the diamond
difference relations and weighted diamond difference relations by assuming
ψ to vary linearly across the cell. These schemes were discussed by
Lathrop with the following criteria in mind: (i) accuracy, i.e., order
of the truncation error, (ii) positivity, i.e., positive sources and bound-
ary fluxes should yield positive fluxes throughout the cell. To these
criteria could be added the requirements that the scheme should be simple,
i.e., involve a small number of arithmetic operations, and easily general-
izable to other geometries.

The equation considered by Lathrop is

$$\mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \textstyle\sum_t \psi(x,y,\mu,\eta) = Q(x,y,\mu,\eta), \tag{25}$$

where the domain of the equation is the rectangle $R = \{(x,y): 0 \leq x \leq \Delta x,$
$0 \leq y \leq \Delta y\}$; μ and η are the x- and y-components (direction cosines) of the

direction vector $\underset{\sim}{\Omega}$. It is assumed that μ and η are both positive, and that the flux ψ is known on the left and bottom edges of R,

$$\psi(0,y,\mu,\eta) = \psi_L(y,\mu,\eta), \qquad \psi(x,0,\mu,\eta) = \psi_B(x,\mu,\eta).$$

The problem then is to find the flux along the right and top edges of R, $\psi_R \equiv \psi(\Delta x,y,\mu,\eta)$ and $\psi_T \equiv \psi(x,\Delta y,\mu,\eta)$, respectively, and some average flux within the cell, $\psi_{cell} \equiv \psi(\overline{x},\overline{y},\mu,\eta)$, from which the source term $Q \equiv Q(\psi,S)$ can be calculated.

In terms of these fluxes, the balance relation that should be satisfied for any finite difference scheme, reads

$$\mu \frac{\psi_R - \psi_L}{\Delta x} + \eta \frac{\psi_T - \psi_B}{\Delta y} + \sum_t \psi_{cell} = Q_{cell}. \qquad (26)$$

a. Step difference scheme. ψ is assumed to be constant throughout R,

$$\psi_L = \psi_B = \psi_R = \psi_T = \psi_{cell}.$$

This scheme is positive. Its truncation error, however, is of less than second order.

b. Diamond difference scheme. ψ is assumed to be linear throughout R, flux averages are evaluated at the midpoints of the respective intervals,

$$\psi_L + \psi_R = \psi_B + \psi_T = 2\psi_{cell}.$$

This scheme has a truncation error which is of second order in (x,y)-geometry only. The scheme is not positive.

c. Weighted diamond difference scheme. As with the previous scheme, ψ is assumed to be linear throughout R. However, the points where the flux averages are evaluated are determined in such a way that the scheme becomes positive,

$$X \, \psi_R + (1-X)\psi_L = \psi_{cell},$$

$$Y \, \psi_T + (1-Y)\psi_B = \psi_{cell}.$$

This scheme has a truncation error which is of second order if and only if $X = Y = \frac{1}{2}$ (diamond difference scheme). It is positive if and only if $X = Y = 1$ (step difference scheme).

      d. <u>Variable weighted difference schemes.</u> Because positivity cannot be guaranteed with fixed weights (X and Y the same for each rectangle R) one assumes that $X \equiv X(\alpha,\beta)$ and $Y \equiv Y(\alpha,\beta)$, with $\alpha = \sum_t (\Delta x)/\mu$, $\beta = \sum_t (\Delta y)/\eta$ (α and β are the x- and y-components of the optical mean free path, respectively). Then one chooses X and Y such that the scheme is positive and such that the values of X and Y are as close to $\frac{1}{2}$ as possible (for $X = Y = \frac{1}{2}$, one obtains the diamond difference scheme, which has a second-order truncation error). These requirements lead to a nonlinear optimization problem which is approximately solved by

$$X = \max(X',\tfrac{1}{2}) \qquad \text{with} \qquad X' = 1 - \beta/\alpha(\beta+2),$$

$$Y = \max(Y',\tfrac{1}{2}) \qquad \text{with} \qquad Y' = 1 - \alpha/\beta(\alpha+2).$$

A more accurate difference scheme consistent with positivity is obtained if, in each rectangle, one makes use of the left and bottom edge fluxes, ψ_L and ψ_B,

$$X = 1 - [\beta + \alpha(\psi_B + \beta Q/\textstyle\sum_t)/\psi_L]/\alpha(\beta+2),$$

$$Y = 1 - [\alpha + \beta(\psi_L + Q/\textstyle\sum_t)/\psi_B]/\beta(\alpha+2).$$

These schemes are positive. However, their truncation errors are not of second order.

e. <u>Higher-order difference schemes</u>. If one assumes that ψ is bi-quadratic in x and y (six unknown coefficients) and evaluates this function at the midpoints of the four edges of R, one obtains two equations for the unknown coefficients from ψ_L and ψ_B and four more equations by requiring that Eq. (25) be satisfied at the corners of R. One thus obtains the diamond difference scheme with a modified source term. This scheme has a truncation error which is at least of second order. It is not positive; however, Lathrop conjectures that this procedure may be used to generate a positive scheme that has a truncation error of second order, in the same way as the weighted difference scheme was generalized from the diamond difference scheme.

These theoretical results were confirmed by numerical experiments. The accuracy of the step difference scheme is generally poor, whereas the diamond difference scheme converges rapidly as the mesh size is decreased. We will come back to these results in the next section.

C. Discrete Ordinates Techniques Based on the Normal Form of the Transport Equation

Approximation procedures for solving the transport equation can be based on either the standard form, Eq. (5), or the normal form, Eq. (6), of the equation. Having discussed the literature on approximation procedures based on the standard form in the previous section, we now turn to a discussion of the literature on approximation procedures based on the normal form.

1. Techniques in which the discrete ordinates are coupled to the spatial mesh

With the transport equation in its normal form it is feasible to develop discrete ordinates techniques in which the set of discrete directions $\{\Omega_k\}$ is coupled with the spatial mesh. One then solves the transport equation by numerically integrating along characteristics. As the characteristics are straight lines, the arithmetic is considerably simplified.

An early proponent of the idea of coupling the discrete ordi-
nates with the spatial mesh was Bareiss,[5] who proposed the method to
integrate the transport equation for arrays of hexagonal cylinders. No
complete analysis was given, though, and a procedure based on these
ideas has never been implemented.

A successful attempt to base a three-dimensional discrete
ordinates approximation on the normal form of the transport equation in
which the discrete directions are coupled to the spatial mesh has recently
been reported by Wagner, et al.[52] The approximation was developed for
arrays of rectangular parallelepipeds; the mesh structure was such that
the distance between two successive mesh points was the same in each of
the three coordinate directions. The neutron flux in a mesh cell was
described in terms of the 14 fluxes in the discrete directions obtained
by connecting the center of the cell with the centers of the 14 neighbor-
ing cells. (An obvious extension of the set of discrete ordinates, which
is not considered by the authors, is obtained if one includes the direc-
tions passing through the midpoints of the edges of a cell. Thus the
number of discrete directions is increased from 14 to 26). The emission
integral was assumed to be constant throughout the cell and equal to its
average value over the cell, so that, in each cell, the unknown fluxes
could be written as linear combinations of the known fluxes and the con-
stant source. The coefficients, which involve exponentials of the optical
distance, were evaluated exactly. The choice of the angular quadrature
weights for the evaluation of the emission integral was based on the re-
quirement that the approximation be consistent with the diffusion approxi-
mation. The scalar flux and the neutron current density were calculated
as weighted averages (over the set of discrete directions) of the averages
along the rays in the various discrete directions.

Although the authors do not present a detailed study of the prop-
erties of the numerical approximation, the results obtained with the
three-dimensional multigroup discrete ordinates code 3DT for a simple
configuration (fuel-block reactivity worths) appear very satisfactory.

To conclude the discussion of approximation procedures in which the discrete ordinates are coupled to the spatial mesh, we submit the following discussion.

The accuracy with which the neutron flux can be computed by means of any approximation procedure is ultimately determined by the accuracy with which one can approximate the emission integral. Thus, the choice of a suitable cubature formula is very important. The accuracy of any cubature formula is limited by the number of points at which the integrand is evaluated, i.e., by the number of discrete ordinates. Hence, if the discrete ordinates are tied to the spatial mesh, the accuracy with which the flux is determined depends, ultimately, on the structure of the spatial mesh. In particular, the function to which the approximate ψ converges as spatial quadrature techniques of increasing accuracy are used, does not correspond to the solution of the global problem and, hence, an approximation procedure based on this approach is never a consistent approximation.

Furthermore, by coupling the discrete ordinates to the spatial mesh one imposes severe restrictions on the latter. Only mesh structures of extreme regularity can be handled in this way. In fact, the only possible structures are those periodic arrays of rectangular prisms generated by the regular tessellations of the plane. This limitation is clearly undesirable from a practical point of view.

2. Techniques in which the discrete ordinates are not coupled to the spatial mesh

In this and the following paragraphs we survey the discrete ordinates techniques which are based on the normal form of the transport equation and in which the discrete ordinates are not coupled to the spatial mesh. The first authors who formulated such a discrete ordinates technique were Keller and Wendroff,[53] and Richtmyer.[30,54] Their studies are limited to one-dimensional geometries.

Keller and Wendroff discuss the case of time-dependent neutron transport in systems which spherical symmetry. The interval $[-1,1]$ of

the angular variable μ is divided into k intervals of equal length $\Delta\mu = 2/k$ and the continuous transport equation is replaced by the following system of discrete ordinates equations,

$$\left(\frac{1}{v}\frac{\partial}{\partial t} + a_k\frac{\partial}{\partial r}\right)(\psi_k + \psi_{k-1}) + \left(\Sigma_t + \frac{b_k}{r}\right)\psi_k$$

$$+ \left(\Sigma_t - \frac{b_k}{r}\right)\psi_{k-1} = Q_k + Q_{k-1} \qquad k = 0,1\ldots K, \qquad (27)$$

with $\mu_k = -1 + k\Delta\mu$ $(k=1\ldots K)$; $a_o = -1$, $a_k = \frac{1}{2}(\mu_k + \mu_{k-1})$ $(k=1\ldots K)$; $b_o = 0$, $b_k = (2/\Delta\mu)[1 - \frac{1}{4}(\mu_k + \mu_{k-1})^2]$ $(k=1\ldots K)$; $\psi_{-1} = Q_{-1} = 0$. Notice that the coefficients a and b are different from the corresponding coefficients in Carlson's discrete ordinates equations. The emission integral is evaluated by means of the trapezoidal rule. The equations (27) are in the normal form and can be integrated along the characteristics, which are straight lines in the (r,t)-plane. Integrating from a point P_k to a point Q along the kth characteristic we obtain a system of integral equations of the form

$$(\psi_k + \psi_{k-1})_Q = (\psi_k + \psi_{k-1})_{P_k}$$

$$+ \int_{P_k}^{Q} [Q_k + Q_{k-1} - (\Sigma_t + \frac{b_k}{r})\psi_k - (\Sigma_t - \frac{b_k}{r})\psi_{k-1}]\frac{ds_k}{D_k}$$

$$k = 0\ldots K, \qquad (28)$$

or, alternatively,

$$(\psi_k + \psi_{k-1})_Q = (\psi_k + \psi_{k-1})_{P_k} \exp\left\{-\int_{P_k}^{Q}(\Sigma_t + \frac{b_k}{r})\frac{ds_k}{D_k}\right\}$$

$$+ \int_{P_k}^{Q}[Q_k + Q_{k-1} + \frac{2b_k}{r}\psi_{k-1}]\exp\left\{-\int_{s_k}^{Q}(\Sigma_t + \frac{b_k}{r})\frac{ds_k'}{D_k}\right\}\frac{ds_k}{D_k},$$

$$(29)$$

where s_k is the arc-length along the kth characteristic and $D_k = (a_k^2 + 1/v^2)^{1/2}$. The equations (28) and (29) are discretized by placing a uniform mesh over the rectangle $\{(r,t): 0 \leq r \leq R, 0 \leq t \leq T\}$. The integrals are evaluated by a modified trapezoidal rule. For example, if we abbreviate the expression in brackets under the integral sign by $\phi_{k-1/2}$, then the integral in Eq. (29) is approximated by $\phi_{k-1/2}(P_k')(\Delta s_k/D_k)$, where Δs_k is the distance between P_k and Q measured along the kth characteristic and P_k' is some point on the characteristic segment from P_k to Q. The other integrals are approximated in a similar manner. The points Q are identified with the mesh points, P_k is taken to be the first inter-section of a mesh line (either horizontal or vertical) with the kth characteristic through Q (traversed in the backward direction). Linear interpolation is used between the mesh points. To approxi-mate $\phi_{k-1/2}(P_k')$ the authors use the average of $Q_k + Q_{k-1}$ along the cell diagonal which passes through the mesh point Q and is nearest to the kth characteristic, and the average of $(\zeta_t + b_k/r)\psi_k + (\zeta_t - b_k/r)\psi_{k-1}$ along the kth characteristic between P_k and Q. The integral equations (29) are treated in an analogous manner. The exponentials are approximated by linear expressions which have posi-tive coefficients. The authors show that under vacuum-type boundary conditions the resulting system of linear algebraic equations for the approximate fluxes at the mesh points admits a unique solution which can be obtained iteratively. The system is unconditionally stable and the solution converges to the solution of Eq. (27) if the mesh size goes to zero. The approximation procedure has been applied successfully to some problems of radiative transfer.

Richtmyer also studied the time-dependent transport equa-tion in spherical geometry (homogeneous medium with isotropic scat-tering). Instead of the variables r and μ, he used x and y, where $x = r\mu$ and $y = r\sqrt{1-\mu^2}$. Thus, the rectangular cylinder $\{(r,\mu,t): 0 \leq r \leq R, -1 \leq \mu \leq 1, t \geq 0\}$ is mapped onto the semicircular cylinder $\{(x,y,t): x^2 + y^2 \leq R^2, y \geq 0, t \geq 0\}$. With these variables the transport equation is

$$\left(\frac{1}{v}\frac{\partial}{\partial t} + \frac{\partial}{\partial x} + \Sigma_t\right)\psi(x,y,t) = Q(r,t) \quad \text{with} \quad r = \sqrt{x^2+y^2} \,. \tag{30}$$

If the sphere is embedded in a vacuum, the boundary condition is

$$\psi(x,y,t) = 0 \quad \text{for} \quad x^2+y^2 = R^2, \quad y \geq 0, \quad x \leq 0.$$

The point (x,y,t) representing a neutron moves in the plane $y =$ constant in the direction of increasing x with the constant speed v until a collision occurs, at which time the representative point jumps to some other point on the same semicircle, (x',y',t') say, from which it then continues to move in the plane $y = y'$ in the direction of increasing x with the same speed v. If a neutron escapes from the system it crosses the surface of the cylinder at a point (x,y,t) with $x > 0$. A three-dimensional orthogonal net of mesh points (x_i,y_j,t_n) is imposed on the semicircular cylinder such that, in each coordinate direction, the mesh points are uniformly distributed and such that the mesh spacings in the x- and t-directions have a ratio which is equal to the neutron speed, v. Thus, because the derivative with respect to x appears in the equation, but not that with respect to y, the integration is along the paths which the neutrons follow between collisions. The discrete ordinates equations in this case are

$$\frac{1}{\Delta x}(\psi_{i+1,j}^{n+1} - \psi_{i,j}^{n}) + \frac{1}{2}\Sigma_t(\psi_{i+1,j}^{n+1} + \psi_{i,j}^{n}) = Q^{n+1/2}(r_{i+1/2,j}), \tag{31}$$

where $\psi_{ij}^{n} = \psi(x_i,y_j,t_n)$, $r_{ij} = \sqrt{x_i^2+y_j^2}$, and where $Q^{n+1/2}(r)$ is an approximate value of $Q(r,t)$ for time $t_{n+1/2} = (n+1/2)\Delta t$, to be obtained by an iterative procedure. The truncation error of this procedure is $O((\Delta t)^2)$.

Bennett[55] investigated a discrete ordinates approximation based on the normal form, Eq. (6), to solve the transport equation (with isotropic scattering) in rectangular (x,y)-geometry. An orthogonal mesh was imposed on the domain of the equation. The flux was evaluated at each mesh point for a set of discrete ordinates $\{\Omega_k = (\theta_k,\phi_k)\}$ which was chosen in such a way that the $\cos\theta_k$ corresponded to the zeros of the Legendre polynomials and the ϕ_k were uniformly spaced in the interval $[0,2\pi]$. The

angular cubature weights are not specified in the reference. The directional derivative $\partial/\partial s$ along the kth characteristic was approximated by a first-order difference along the same characteristic. Linear interpolation was used between the mesh points to calculate the flux along the edge of a mesh cell. The collision density $\sum_t \psi$ and the scalar flux ϕ were averaged along each characteristic. A few parametric studies were conducted by means of a research computer code, TXY01, to determine the accuracy of the method in solving the transport equation in a purely absorbing slab and in a two-dimensional rectangular cell. According to Hageman,[56] the results were not promising enough, however, to justify a further investigation of the approximation procedure.

3. Positivity vs. accuracy

We now come back to the article by Lathrop[51] which we discussed earlier in Section B, Subsection 5 of this chapter. We recall that the author studied various difference schemes which had been proposed in the literature for the solution of the transport equation in (x,y)-geometry. In the previous section we discussed his findings with respect to the positivity and accuracy of those difference schemes which are based on the standard form of the transport equation. In this subsection we discuss those schemes which are based on the normal form of the equation. We will use the same notation as in Section B, Subsection 5.

If one assumes that the spatial mesh is sufficiently fine, so that the cross sections do not vary across the rectangular cell R, the integral equation (7), which is obtained by integrating the normal form of the transport equation, Eq. (6), along a characteristic, reduces to

$$\psi = \psi^o \exp\left(-\sum_t s\right) + \int_o^s Q \exp\left[-\sum_t (s-s')\right] ds', \tag{32}$$

where ψ^o is the flux on the boundary, s is the distance from the boundary to the point at which ψ is evaluated and s' is the point at which Q is evaluated. The postulated behavior of the flux ψ throughout a

mesh cell is used in conjunction with the discrete ordinates form of the integral equation (6) to express the unknown fluxes (ψ_R and ψ_T) in terms of the known fluxes (ψ_L and ψ_B). Hence, in contrast to the difference schemes based on the standard form of the transport equation, difference schemes based on the normal form of the equation are not necessarily conservative in the sense that they lead to flux values which satisfy Eq. (26).

a. Step function characteristic scheme. ψ_L and ψ_B (the known fluxes along the left and bottom edges of the rectangular domain R) as well as Q are assumed to be constant in R. Then ψ_R and ψ_T are determined from the equations

$$\psi_R = Q/\Sigma_t + (\psi_B - Q/\Sigma_t)(1 - e^{-\beta})/\beta,$$

$$\psi_T = Q/\Sigma_t + (\psi_L - Q/\Sigma_t)(1 - e^{-\beta})/(\rho\beta)$$

$$+ (\psi_B - Q/\Sigma_t)(1 - 1/\rho)e^{-\beta},$$

for $\rho > 1$, and

$$\psi_R = Q/\Sigma_t + (\psi_L - Q/\Sigma_t)(1 - \rho)/\beta$$

$$+ (\psi_B - Q/\Sigma_t)\rho(1 - e^{-\alpha})/\alpha,$$

$$\psi_T = Q/\Sigma_t + (\psi_L - Q/\Sigma_t)(1 - e^{-\alpha})/\alpha,$$

for $\rho < 1$. In these expressions α, β and ρ denote the abbreviations

$$\alpha = \Sigma_t(\Delta x/\mu), \qquad \beta = \Sigma_t(\Delta y/\eta), \qquad \rho = \alpha/\beta. \qquad (33)$$

The value of ρ determines where the characteristic through the lower left corner intersects the top or right edge of R.

This scheme is positive and conservative. However, its truncation error is not of second order.

b. <u>Wendroff's characteristic scheme</u>. (This scheme has been suggested for the numerical solution of the equation of radiative transfer.) The average fluxes are evaluated at the midpoints of the respective intervals. Consider a characteristic which passes through the center of R. Its projection on the (x,y)-plane intercepts the line through the midpoints of the left and bottom edge of R at a point Q and the line through the midpoints of the right and top edges of R at a point P. Let ψ_Q be the flux at Q obtained by linear interpolation from ψ_L and ψ_B,

$$\psi_Q = \Delta s[(\mu/\Delta x)\psi_L + (\eta/\Delta y)\psi_B], \quad \Delta s = [(\mu/\Delta x) + (\eta/\Delta y)]^{-1}. \tag{34}$$

Then, from the integral equation (32) we find

$$\psi_P = \psi_Q e^{-\Sigma_t \Delta s} + (Q/\Sigma_t)(1 - e^{-\Sigma_t \Delta s}). \tag{35}$$

In turn, ψ_P can be interpreted as the flux at P obtained by linear interpolation from ψ_R and ψ_T,

$$\psi_P = \Delta s[(\mu/\Delta x)\psi_R + (\eta/\Delta x)\psi_T]. \tag{36}$$

One more relation is needed to find the unknowns ψ_R and ψ_T. For example, one may choose

$$\psi_R + \psi_L = \psi_B + \psi_T.$$

The scheme thus obtained has a truncation error which is of second order; moreover, the scheme is conservative. However, it is not positive.

c. <u>Woods-Carlson characteristic scheme</u>. This scheme is a generalization of Wendroff's scheme. Again, all averages are evaluated at the midpoints of the respective intervals. Noting that in Wendroff's scheme ψ_R and ψ_T are obtained as linear combinations of ψ_L and ψ_B one may write, generally,

$$\begin{pmatrix} \psi_R \\ \psi_T \end{pmatrix} = A \begin{pmatrix} \psi_L \\ \psi_B \end{pmatrix} + (Q/\Sigma_t)(1 - e^{-\Sigma_t \Delta s}),$$

where A is a 2×2 matrix which may be determined by the following criteria: (i) if $\psi_L = \psi_B$, then $\psi_R = \psi_T$; (ii) if $\psi_L = \psi_B = Q/\Sigma_t$, then $\psi_R = \psi_T = Q/\Sigma_t$; (iii) Eqs. (34) through (36) must be satsified. This yields three linearly independent equations. Woods and Carlson suggest taking

$$A_{WC} = \begin{pmatrix} (1-\rho)\tau & \tau \\ \tau & 0 \end{pmatrix} \text{ for } \rho < 1, \quad A_{WC} = \begin{pmatrix} 0 & \tau \\ \tau/\rho & (1-1/\rho)\tau \end{pmatrix} \text{ for } \rho > 1, \quad (37)$$

where $\tau = \exp(-\Sigma_t \Delta s)$ and ρ is defined by Eq. (33). The choice of Eq. (37) should be compared with the following expression in Wendroff's scheme,

$$A_W = \begin{pmatrix} (\tau-\rho)/(1+\rho) & \rho(1+\tau)/(1+\rho) \\ 2/(1+\rho) & (\rho\tau-1)/(1+\rho) \end{pmatrix}.$$

The scheme (37) is positive and conservative. However its truncation error is worse than second order.

d. Corner-point characteristic schemes. In these schemes the flux is evaluated at the four corners of the rectangular domain R and is assumed to vary linearly along the edges. An example of such a scheme is the scheme developed by Bennett and described in the previous subsection (Subsection 2). This scheme is positive. Its truncation error might be of second order. The scheme is not conservative.

As mentioned before, in Section B, Subsection 5, Lathrop also performed numerical experiments with various difference schemes. It was observed that all characteristic schemes gave essentially similar

results and that these results agreed roughly with those obtained with the weighted diamond difference scheme.

Summarizing Lathrop's findings we can say that, of all the positive schemes investigated, the variable weighted diamond difference scheme is the most attractive; all positive schemes are less accurate than the diamond difference scheme; for global accuracy, fix-up schemes which ensure a minimum change from the diamond difference scheme are to be preferred to the strictly positive schemes because of easy implementation.

IV. REFERENCES

1. T. Roşescu, "Neutron transport theory," IFA-FR-48 (Vol. I),
   IFA-FR-51 (Vol. II). Academy of the Socialist Republic of
   Rumania, Institute of Atomic Physics, Bucharest, 1965, 1966.

2. W. L. Hendry, K. D. Lathrop, S. Vandervoort, J. Wooten, "Biblio-
   graphy on neutral particle transport theory," LA-4287-MS, Los
   Alamos Scientific Laboratory, 1970.

3. S. Chandrasekhar, Radiative transfer, Oxford, 1950.

4. B. Davison, Neutron transport theory, Oxford, 1957.

5. E. H. Bareiss, "A Survey and Classification of Transport Theory
   Calculation Techniques," in: Proc. United Nations Int. Conf. on
   Peaceful Uses of Atomic Energy, 16 P/639, Geneva, 1958.

6. H. Greenspan, C. N. Kelber, D. Okrent (Eds.), Computing Methods
   In Reactor Physics, Gordon and Breach, New York (N.Y.), 1968.

7. B. G. Carlson, K. D. Lathrop, "Transport Theory - The method of
   discrete ordinates," Chapter 3 of Ref. 6.

8. E. M. Gelbard, "Spherical harmonics method: P_L and double-P_L
   method," Chapter 4 of Ref. 6.

9. R. B. DeBar, "Difference equations for the Legendre polynomial
   representation of the transport equation," J. Comp. Phys. 2 (1967),
   197.

10. C. Maeder, "A three-dimensional P_N spherical harmonics theory in
    cylindrical geometry," Nucl. Sci. and Eng., 33 (1968), 128.

11. T. Juillerat, "A three-dimensional multigroup P_L-theory with axially
    variable parameters," Nukleonik 12 (1969), 117.

12. R. C. Gast, "The two-dimensional, quadruple P_0 and P_1 approximations,"
    WAPD-TM-274, Bettis Atomic Power Laboratory (1961).

13. R. B. DeBar, "Truncation of the spherical harmonic expansion of the
    transport equation," Nucl. Sci. and Eng. 30 (1967), 159.

14. B. Davison, "Transport theory of neutrons," LT-18, Nat. Research
    Council of Canada, 1947.

52

15. G. C. Pomraning, "A generalized P-N approximation for neutron transport problems," Nukleonik $\underline{6}$ (1965), 348.

16. G. C. Pomraning, "An asymptotically correct approximation to the multidimensional transport equation," Nucl. Sci. and Eng. $\underline{22}$ (1965), 328.

17. J. A. Davis, "Transport error bounds via P_N approximation," Nucl. Sci. and Eng. $\underline{31}$ (1968), 127.

18. A. J. Buslik, "Extremum variational principles for the monoenergetic neutron transport equation with arbitrary adjoint source," Nucl. Sci. and Eng. $\underline{35}$ (1969), 303.

19. G. Ya. Rumyantsev, "Boundary conditions in the spherical harmonics method," Reactor Sci. and Techn. $\underline{16}$ (1962), 111.

20. F. D. Federighi, "Vacuum boundary conditions for the spherical harmonics method," Nukleonik, $\underline{6}$ (1964), 277.

21. K. M. Dede, Z. T. Bödy, "Vacuum boundary conditions for multidimensional spherical harmonics method," Nukleonik $\underline{8}$ (1966), 388.

22. T. Toivanen, "A selfadjoint variational principle for deriving vacuum and interface boundary conditions in the spherical harmonics method," Nucl. Sci. and Eng. $\underline{25}$ (1966), 275.

23. J. A. Davis, "Variational vacuum boundary conditions for a P_N approximation," Nucl. Sci. and Eng. $\underline{25}$ (1966), 189.

24. J. A. Davis, "Continuity conditions for a homogeneous or heterogeneous P_N approximation," Nucl. Sci. and Eng. $\underline{27}$ (1967), 542.

25. J. P. Church, "Solving the transport equation in heterogeneous media using first-flight Green's functions for homogeneous media," Nucl. Sci. and Eng. $\underline{21}$ (1965), 49.

26. A. A. Aswad, G. R. Dalton, "Integral transport theory," Nucl. Sci. and Eng. $\underline{24}$ (1966), 49.

27. T. Carlvik, "Integral transport theory in one-dimensional geometries," Nukleonik $\underline{9}$ (1967), 104.

28. E. P. Wigner, <u>Group Theory and its Application to the Quantum Mechanics of Atomic Spectra</u>, Academic Press, New York, 1959.
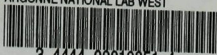
52

29. B. G. Carlson, "A method of moments for solving the neutron trans-
    port equation," LA-3060, Los Alamos Scientific Laboratory, 1965.

30. R. Richtmyer, _Difference methods for initial-value problems_, Inter-
    science, 1957.

31. G. Goertzel, "The method of discrete ordinates," Nucl. Sci. and
    Eng. 4 (1958), 4.

32. R. Gast, "On the equivalence of the spherical harmonics method and
    the discrete ordinate method using Gauss quadrature for the Boltz-
    mann equation," WAPD-TM-118, Bettis Atomic Power Laboratory, 1958.

33. B. G. Carlson, K. D. Lathrop, "Moments equations and equivalent
    discrete ordinates equations," Trans. Am. Nucl. Soc. 8 (1965), 487.

34. K. D. Lathrop, N. S. Demuth, "Biorthogonal angular expansion of
    the Boltzmann transport equation," LA-3617, Los Alamos Scientific
    Laboratory, 1965.

35. K. D. Lathrop, N. S. Demuth, "Biorthogonal polynomial expansion of
    the two-dimensional transport equation," Nucl. Sci. and Eng. 32
    (1968), 120.

36. M. F. Didon, "Etude de certaines fonctions analogues aux fonctions
    X_n de Legendre, etc.," Ann. Scient. de l'Ecole Norm. Sup., 5
    (1868), 229.

37. K. D. Lathrop, "Ray effects in discrete ordinates equations,"
    Nucl. Sci. and Eng. 32 (1968), 357.

38. B. G. Carlson, "Solution of the transport equation by S_n approxi-
    mations," LA-1599, Los Alamos Scientific Laboratory, 1953.

39. B. G. Carlson, "Numerical solution of neutron transport problems,"
    in: _Nuclear Reactor Theory_, vol. XI, Am. Math. Soc., Proc. of
    Symp. in Appl. Math., Providence (R.I.), 1961.

40. C. E. Lee, "The discrete S_n approximation to transport theory,"
    LA-2595, Los Alamos Scientific Laboratory, 1962.

41. H. B. Keller, "Approximate solutions of transport problems. II.
    Convergence and applications of the discrete ordinate method,"
    J. Soc. Ind. Appl. Math. 8 (1960), 43.

42. H. B. Keller, "On the pointwise convergence of the discrete ordinate method," J. Soc. Ind. Appl. Math. $\underline{8}$ (1960), 560.

43. H. B. Keller, "Convergence of the discrete ordinate method for the anisotropic scattering transport problem," in: Symposium, Provisional Int'l. Computation Centre, Birkhäuser Verlag, Basel, 1960.

44. B. Wendroff, "On the convergence of the discrete ordinate method." J. Soc. Ind. Appl. Math. $\underline{8}$ (1960), 508.

45. K. D. Lathrop, B. G. Carlson, "Numerical solution of the Boltzmann transport equation," J. Comp. Phys. $\underline{1}$ (1967), 173.

46. I. P. Grant, "Numerical analysis of discrete ordinate methods," J. Comp. Phys. $\underline{2}$ (1968), 381.

47. I. P. Grant, G. Hunt, "Discrete space theory of radiative transfer," Proc. Roy. Soc., London $\underline{A313}$ (1969)- 183,199.

48. J. A. Davis, L. A. Hageman, R. B. Kellogg, "Singular difference approximation for the discrete ordinate equations in x-y geometry," Nucl. Sci. and Eng. $\underline{29}$ (1967), 237.

49. W. H. Reed, K. D. Lathrop, "Truncation error analysis of finite difference approximations to the transport equation," Nucl. Sci. and Eng. $\underline{41}$ (1970), 237.

50. S. Kaplan, "A new derivation of discrete ordinate approximations," Nucl. Sci. and Eng. $\underline{34}$ (1968), 76.

51. K. D. Lathrop, "Spatial differencing of the transport equation: positivity vs. accuracy," J. Comp. Phys. $\underline{4}$ (1969), 475.

52. M. R. Wagner, D. A. Sargis, S. C. Cohen, "A numerical method for the solution of three-dimensional neutron transport problems," Nucl. Sci. and Eng. $\underline{41}$ (1970), 14.

53. H. B. Keller, B. Wendroff, "On the formulation and analysis of numerical methods for time dependent transport equations," Comm. Pure and Appl. Math. $\underline{10}$ (1957), 567.

54. R. D. Richtmyer, "A numerical method for the time-dependent transport equation," NYO-7696, AEC Computing Facility, Institute of Mathematical Sciences, New York University, 1957.

55. J. H. Bennett, "TXY01: A one-group transport program for x-y geometry," WAPD-TM-842, Bettis Atomic Power Laboratory, 1964.

56. L. Hageman, private communication (1970).